

Problema 7

recordemos $\hat{f}(i) = \hat{h}(i) + \sum_b^{occ} \hat{J}_b(i) - \hat{K}_b(i)$

$$\hat{f} = \hat{h}(r) + \sum_b^{occ} (\hat{J}_b - \hat{K}_b)$$

\hat{J}_ψ y \hat{K}_ψ se definen en la base que los escribimos

$$\hat{J}_\psi \rightarrow \langle c | \hat{J}_\psi | d \rangle = \langle c\psi | d\psi \rangle$$

$$\hat{K}_\psi \rightarrow \langle c | \hat{K}_\psi | d \rangle = \langle c\psi | \psi d \rangle$$

Para el H_2 , occ son $\{\bar{1}, \bar{2}\}$

$$\hat{f} = \hat{h}(r) + \hat{J}_{\bar{1}} - \hat{K}_{\bar{1}} + \hat{J}_{\bar{2}} - \hat{K}_{\bar{2}}$$

y buscamos $\langle 1 | \hat{f} | 1 \rangle$, $\langle 1 | \hat{f} | 2 \rangle = \langle 2 | \hat{f} | 1 \rangle = 0$

$$\langle 2 | \hat{f} | 2 \rangle$$

y fuere ver que $E_1 \equiv f_{11}$ / $E_2 \equiv f_{22}$ / $\begin{matrix} \text{o sea } \hat{f} \\ \text{diagonal en esta} \\ \text{base.} \end{matrix}$

$$\langle 2 | \hat{f} | 1 \rangle = \langle 2 | \hat{h} | 1 \rangle + \langle 2 | J_1 | 1 \rangle - \langle 2 | K_1 | 1 \rangle \\ + \langle 2 | J_{\bar{1}} | 1 \rangle - \langle 2 | K_{\bar{1}} | 1 \rangle$$

$$= h_{12} + \langle 2 | J_1 | 1 \rangle - \langle 2 | K_1 | 1 \rangle \\ + \langle 2 | J_{\bar{1}} | 1 \rangle - \langle 2 | K_{\bar{1}} | 1 \rangle$$

$$= h_{12} + \langle 2 | J_1 | 1 \rangle \leftarrow \text{se zulten}$$

$$\langle 1 | \hat{f} | 1 \rangle = \epsilon_1 = h_{11} + \langle 1 | J_1 | 1 \rangle$$

$$\langle 2 | \hat{f} | 2 \rangle = \epsilon_2 = h_{22} + 2 \langle 2 | J_1 | 2 \rangle - \langle 2 | K_1 | 2 \rangle$$

↓

$$\langle 2 | \hat{f} | 2 \rangle = h_{22} + \langle 2 | J_1 | 2 \rangle - \langle 2 | K_1 | 2 \rangle \\ + \langle 2 | J_{\bar{1}} | 2 \rangle - \langle 2 | K_{\bar{1}} | 2 \rangle$$

$$= h_{22} + \langle 2 | J_1 | 2 \rangle - \langle 2 | K_1 | 2 \rangle \\ + \langle 2 | J_{\bar{1}} | 2 \rangle - \langle 2 | K_{\bar{1}} | 2 \rangle$$

$$= h_{22} + 2 \langle 2 | J_1 | 2 \rangle - \langle 2 | K_1 | 2 \rangle \\ + \langle 2 | J_{\bar{1}} | 2 \rangle - \langle 2 | K_{\bar{1}} | 2 \rangle \quad \checkmark$$